Applications Breakout Notes

Questions

- Goal: Identify initial pool of apps which are good candidates to run on BG/L
  1. Which consortium members are willing to commit to porting one or more applications?
  2. What are needs of these apps – libraries, tools, kernel support, hardware, optimized mpi, etc.? Prioritize needs for software and hardware groups.
  3. How to organize user support community to share experiences, resources, collect benchmarks, etc?
  4. How to accelerate path to using hardware as it becomes available

Issues from FLASH port

- Memory overflow error reporting/handling should be improved, especially when using automatic f90 arrays. Just getting seg errors is not good.
- Compiler-based double Hummer (-440d) gives < 3 % improvement (Compiler should generate better Double Hummer code)
- Sqrts, divs need to be improved. (MASS, MASSV)
- “Easy to use MPI profiler” was very useful. Should be available to all users.
- Ran code only in heater mode. 3d problem does not fit on 512 nodes. Co-proc mode didn’t work

Who Has Applications that they want to Port to BG/L NOW!

- U. of Utah: Structure Combustion Model - need threads but can use user threads. Hbrid MPI/OpenMP code
- Oakridge: LSMS Electronic Structure Code. Already on SP. Should scale well and needs this machine. Runs on X1 but is more suitable for BG/L. # of atoms = Number of processors
- Yue Fang Dang – BNL – already has code running on QCDOC – N^(3/2) Ewald.
- Fast Multipole code from NYW. Won Gordon Bell last year.
- MILC code - QCD
- U. of Texas – Hydro Fluid Heat Transfer. Unstructured Grid Code (Graham Carey, Bill Barth).
- NCAR – HOMME code Climate Modeling – Rich Loft. (needs good math libs, need MPI_COMM_NOT_WHOLE_WORLD)
- U. of Illinois – Rocket Motor Simulation.
- UCSF, Protein Structure Prediction and Docking. Ben Webb, John Chodera

Main Obstacles

- REMOTE ACCESS IS A PROBLEM. Rochester could be a place for initial efforts in code porting. Need to have a mechanism in place to do this.
- Publicly available batch queue submission possible?
- Hardware counters do not give useful information.
- Get people with difficult porting problems access to the simulator
- Not hard to find applications –

  GET PEOPLE ACCESS TO THE MACHINE.

Other issues

- Some discussion of the importance of a centralized documentation, performance database (base of of SDSC site?)

Running your code

Current (non-scalable) model:

Email if you want to run apps

- Bob Walkup (walkup@us.ibm.com)
- Gyan Bhanot (gyan@us.ibm.com)